

Capturing Complete Spatial Context in Satellite Observations of Greenhouse Gases

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ABSTRACT

Scientific consensus from a 2015 pre-Decadal Survey workshop highlighted the essential need for a wide-swath (mapping) low earth orbit (LEO) instrument delivering carbon dioxide (CO₂), methane (CH₄), and carbon monoxide (CO) measurements with global coverage. OCO-2 pioneered space-based CO₂ remote sensing, but lacks the CH₄, CO and mapping capabilities required for an improved understanding of the global carbon cycle. The Carbon Balance Observatory (CARBO) advances key technologies to enable high-performance, cost-effective solutions for a space-based carbon-climate observing system. CARBO is a compact, modular, 15-30° field of view spectrometer that delivers high-precision CO₂, CH₄, CO and solar induced chlorophyll fluorescence (SIF) data with weekly global coverage from LEO. CARBO employs innovative immersion grating technologies to achieve diffraction-limited performance with OCO-like spatial (2x2 km²) and spectral ($\lambda/\Delta\lambda \approx 20,000$) resolution in a package that is >50% smaller, lighter and more cost-effective. CARBO delivers a 25- to 50-fold increase in spatial coverage compared to OCO-2 with no loss of detection sensitivity. Individual CARBO modules weigh < 20 kg, opening diverse new space-based platform opportunities.

Keywords: Carbon Dioxide (CO₂), Methane (CH₄), Carbon Monoxide (CO), satellite, remote sensing, wide-field, Low Earth Orbit (LEO), mapping

1. INTRODUCTION

There is an urgent need to better understand and predict the future role of the carbon cycle in the climate system [1]. Changes in atmospheric radiative forcing due to natural and anthropogenic emissions of the greenhouse gases carbon dioxide (CO₂) and methane (CH₄) will likely be the most important driver of climate change in the 21st century. Human activities have caused unprecedented, rapid increases in atmospheric CO₂ and CH₄ concentrations since the beginning of the industrial era [2], with anthropogenic emissions forecasted to increase exponentially through 2050 [3]. Earth System feedbacks reduce or amplify the effects of those emissions on atmospheric concentrations, yet despite decades of research, carbon-climate feedbacks remain poorly quantified. It is critical to understand the relationship between climate forcing from anthropogenic emissions, climate-carbon cycle feedbacks, and the resulting atmospheric CO₂ and CH₄ concentrations in a changing climate [2]. This requires a mechanistic understanding of the global carbon cycle, including quantified space- and time-resolved patterns of anthropogenic emissions, natural sources and sinks, and the key processes controlling them [1]. “What processes control the rate of increase in atmospheric CO₂ and CH₄ and will these change in the future?” is the fundamental question of carbon-climate system science.

To address this question, we are developing the Carbon Balance Observatory (CARBO), a new generation of space-based carbon cycle remote sensing technology. CARBO is designed to measurement requirements that will enable us to significantly improve our understanding of and our ability to predict the likely future trajectory of atmospheric CO₂ and

CH₄. CARBO is a modular wide-swath (15–30° field of view) polarization insensitive spectrometer that will deliver CO₂, CH₄, CO and solar-induced chlorophyll fluorescence (SIF, a proxy for gross photosynthetic carbon uptake and vegetation health [4]) measurements with high accuracy and weekly global coverage at ~2 km spatial resolution from low Earth orbit (LEO, Fig. 1). We exploit advances in immersion grating and electron beam lithography technologies to deliver CARBO's increased capability in a package that is >50% smaller and lighter than the Orbiting Carbon Observatory (OCO-2) instrument. CARBO thus benefits from significant cost savings and increased satellite accommodation opportunities. An instrument with CARBO measurement capabilities is not feasible at a reasonable size and cost using the OCO-2 design strategy.

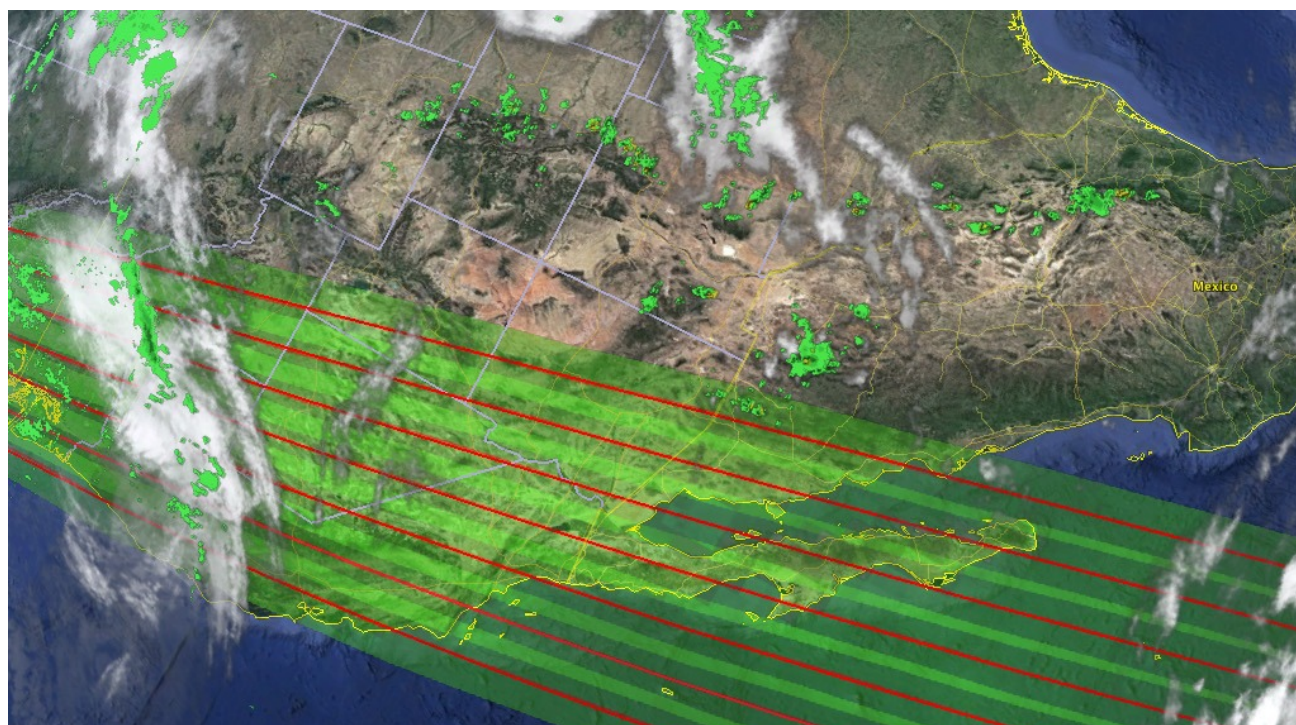


Figure 1. Comparison of OCO-2 (red lines, ~10 km swath) and CARBO (green, 15° FOV) spatial coverage over the western United States for 7 adjacent LEO orbit tracks (~3% of one 16-day repeat cycle). One CARBO 15° FOV module not only increases spatial coverage ~25x vs OCO-2, but the brighter green areas show where adjacent CARBO swaths overlap for repeat sampling.

2. CARBO OBJECTIVES & SCIENCE REQUIREMENTS

A complex interplay of natural and anthropogenic processes controls the atmospheric concentrations of CO₂. Terrestrial ecosystems currently offset ~25% of anthropogenic CO₂ emissions due to a slight imbalance between global terrestrial photosynthesis (gross primary productivity, GPP) and respiration (ER). Understanding what controls GPP and ER is therefore crucial to predicting climate change [5]; however, there is no consensus on the global GPP, and large uncertainties exist in its benchmarking (Fig 2) [6]. GPP and ER fluxes are generally inferred from measurements of CO₂ net ecosystem exchange (NEE = GPP - ER) since there is no way of directly measuring photosynthesis or respiration [5]. Similarly, there are important uncertainties in estimates of the magnitude and distribution of anthropogenic CO₂ emissions [7], and these uncertainties will grow as the fraction of future anthropogenic emissions shifts to developing countries [8]. In fact, circa 2010 uncertainties in anthropogenic emissions dominate the global CO₂ budget [9]. Concurrent measurements of CO₂ and carbon monoxide (CO) have proven a powerful approach for disentangling anthropogenic and combustion emissions from natural fluxes [10–12]. There is thus an urgent need to improve

observation-based CO₂, GPP and CO data sets as well as the representation of key natural and anthropogenic processes within carbon cycle models to accurately estimate the present CO₂ budget and better quantify the future fraction of anthropogenic CO₂ emissions that remain in the atmosphere [6].

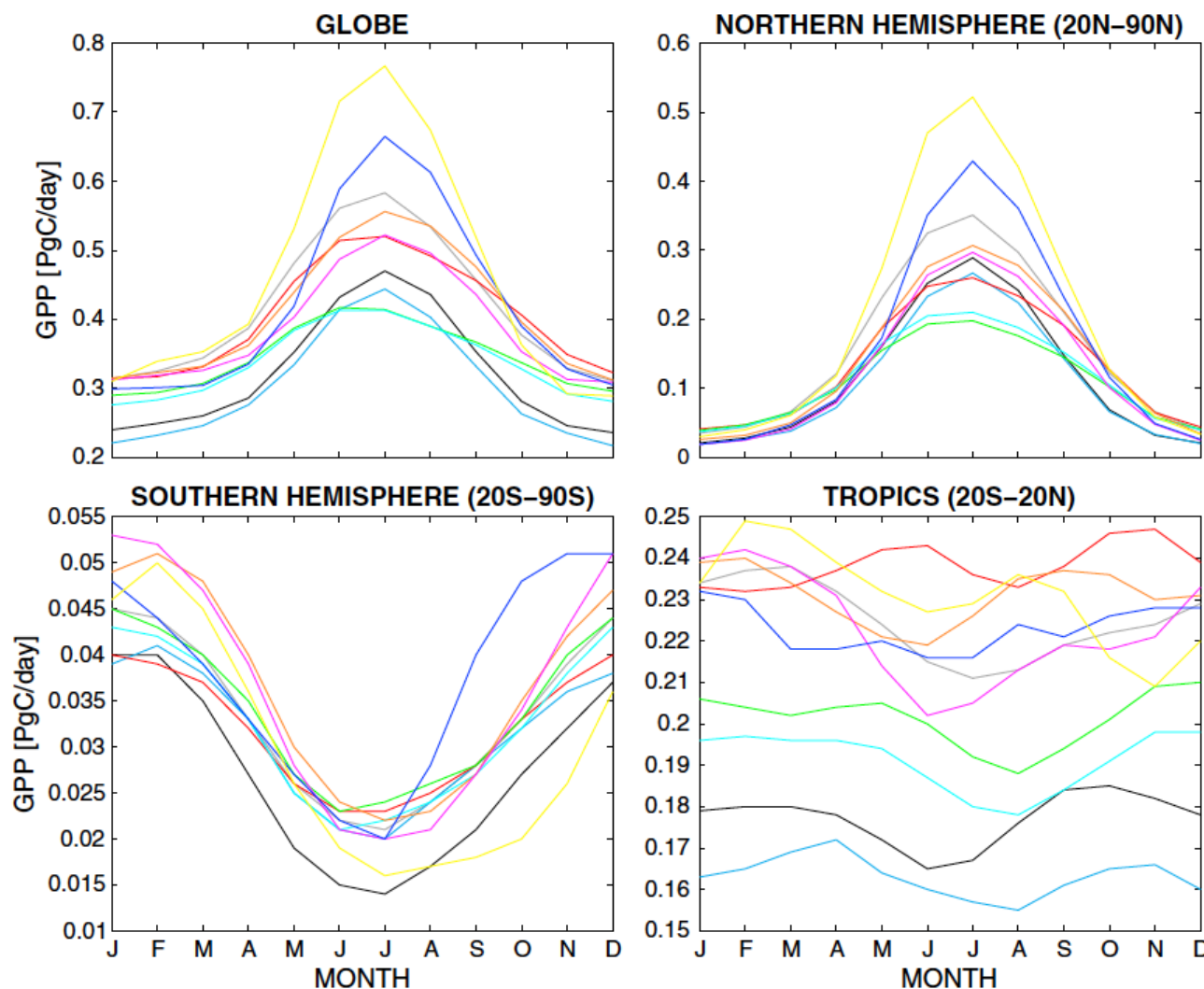


Figure 2. Different models show significant discrepancies in representations of the magnitude, shape and timing of the annual GPP (photosynthesis) cycle [6]. CARBO's enhanced SIF and high-sensitivity CO₂ measurements combined with high spatial resolution and weekly global mapping will revolutionize our understanding of global GPP and photosynthesis.

The processes controlling the global budget of CH₄ (Fig 3), the second most important anthropogenic greenhouse gas, are even more uncertain [13]. Numerous field studies have shown that inventories of anthropogenic CH₄ emissions systematically underestimate observed emissions by 50-100% or more, particularly in major urban areas [14] or from natural gas systems [15]. Concentrations of atmospheric CH₄ had stabilized in the early 2000s, but began abruptly increasing again in 2007 [16]. Changes in CH₄ emissions from tropical wetlands [17], agriculture in Southern Asia [18], and increasing US fugitive emissions [19] have been proposed as the catalyst for this upturn, although the factors responsible for the observed stabilization and renewed rise remain unclear and can not be definitely resolved given uncertainties in the global CH₄ budget [13]. The partitioning of CH₄ emissions by region and process is poorly

constrained by current atmospheric observations and would benefit from denser, more evenly distributed CH_4 concentration data [13].

The current system of global atmospheric CO_2 and CH_4 measurements does not adequately constrain process-based carbon cycle models to allow diagnosis and/or attribution of carbon fluxes with confidence. Improving satellite observations of CO_2 , CH_4 , CO and SIF is necessary to advance our understanding of the carbon cycle, including necessary improvements in process-based models and their ability to predict future atmospheric CO_2 and CH_4 levels [20]. Expert consensus is that this could be achieved with “top-down” estimates of CO_2 and CH_4 surface fluxes monthly at 100 km spatial resolution ($\sim 1^\circ \times 1^\circ$) by combining satellite data with atmospheric inversion models over several annual cycles [20]. CO and SIF measurements enhance CO_2 and CH_4 flux diagnosis and attribution.

Space-based measurements of the column averaged dry air mole fraction (denoted X_{GHG}) retrieved from high-resolution spectroscopic observations of reflected sunlight in near infrared CO_2 and CH_4 bands have the potential to significantly reduce carbon flux uncertainties [21]. OCO-2 (X_{CO_2}) and GOSAT (X_{CO_2} and X_{CH_4}) pioneered this capability, but a much denser observational grid is needed to retrieve estimates of surface fluxes at the required spatial and temporal resolution ($\sim 1^\circ \times 1^\circ$, monthly). Contiguous mapping at high spatial resolution provides the spatial context required to quantify and attribute natural and anthropogenic point sources.

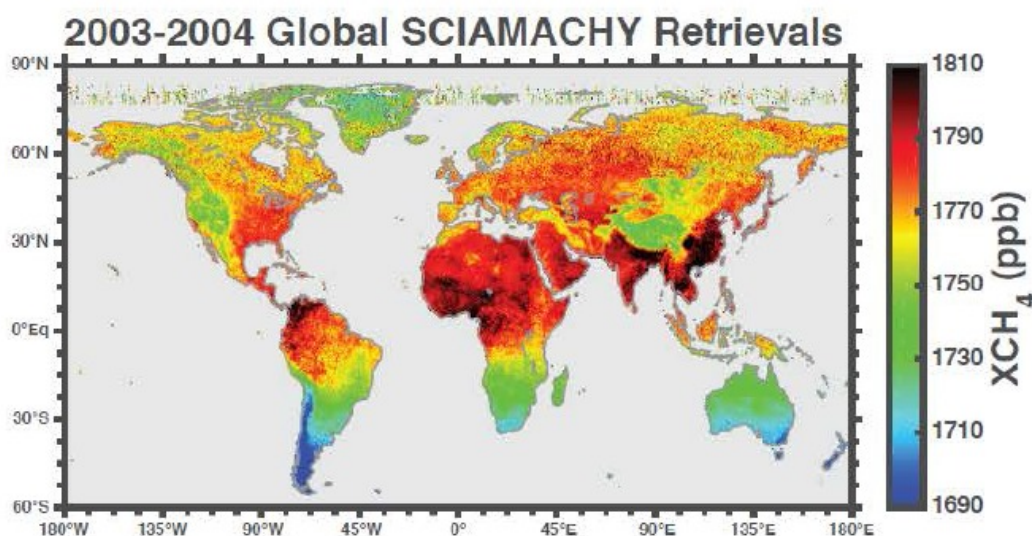


Figure 3. Global X_{CH_4} retrievals from SCIAMACHY required 2 years of averaging to reveal key spatial patterns [23]. CARBO's weekly revisits, high sensitivity and high spatial resolution will yield critical insights on CH_4 temporal dynamics for a mechanistic understanding of the underlying emissions processes.

OCO-2 is a grating spectrometer designed to retrieve CO_2 using three near infrared spectral channels [22]. Its $\sim 3 \text{ km}^2$ nadir spatial resolution maximizes cloud-free observations while its high spectral resolution and signal-to-noise ratio enable an unprecedented 1 ppm X_{CO_2} retrieval precision [21]. OCO-2 is thus optimally suited to sample the global atmospheric CO_2 distribution. However, the OCO-2 swath is only 10 km wide, meaning that it samples only 7% of the Earth's surface and does not provide the critical spatial context information that comes with complete mapping. Furthermore, OCO-2 is polarization sensitive and requires continuous satellite rotation to keep the instrument slit oriented perpendicular to the principal plane. This complicates operations and reduces the effective swath width from 10 km to as little as 1.3 km. Finally, OCO-2 does not measure CH_4 or CO, limiting its effectiveness in carbon flux inversion studies, informed policy decisions, emissions monitoring, etc.

CARBO's wide swath design enables full global mapping at high spatial resolution and weekly revisit times. CARBO's simultaneous CO₂, CH₄, CO and SIF measurements allow us to establish the functional relationships between CO₂, CH₄ and CO fluxes with environmental and biogeochemical controls such as soil moisture, vegetation type/structure, photosynthetic efficiency and vegetation stress [24-25]. These functional relationships enable the mechanistic understanding required to reliably project how major components of the climate-carbon cycle system such as tropical ecosystem exchange [26] or the permafrost carbon feedback [27] will respond to climate change. CARBO's weekly revisits better reveal CO₂, CH₄ and CO spatial gradients since these are more pronounced than monthly or seasonal averages. Complete mapping minimizes representativeness errors in inverse model flux estimates [28] and direct detection of point sources vs. local background, enabling simple emission estimates for sources like power plants, landfills, isolated wetlands, gas exploration, etc. [29]. Without mapping capabilities, detection and quantification of point sources would be fortuitous and defy robust attribution.

2.1 CARBO Performance Requirements

We quantified CARBO instrument performance requirements using our proposed wide-field immersion grating spectrometer design. Radiometric simulations indicate that the CARBO design achieves >90% of the OCO-2 instrument SNR specifications by filling the FPA and enhancing throughput by a factor 1.3-1.5 as a result of immersion grating technology. CARBO's estimated 1.5 ppm single measurement precision X_{CO2} sensitivity is thus similar to OCO-2. We also evaluated performance requirements for X_{CH4}, X_{CO} and SIF. We found that the detection of CO₂ and CH₄ can be combined within a single 1600 nm channel at somewhat lower spectral resolution without loss of accuracy [30]. This way, CO₂ and CH₄ can be measured in one band and the CH₄ proxy retrieval method [10,31] employed. Sensitivity tests showed that the CARBO design (based on radiometric performance estimates of the proposed optical design and Hawaii-class focal plane array detectors like those flown on OCO-2) could achieve 7 ppb X_{CH4} single measurement precision for typical scenes. Sensitivity studies for the 2350 nm region (not shown here) indicate the CARBO design achieves a 5 ppb single measurement precision in X_{CO}. CARBO X_{CO2}, X_{CH4} and/or X_{CO} detection sensitivities are consistent with pre-flight estimates from instruments with similar SNR and spectral resolution such as TropOMI [32] and CarbonSat [33].

CARBO introduces a major improvement in SIF detection sensitivity by extending the O₂ A-band spectral range to 740 nm. This improves the single measurement precision by 3x compared to sensors limited to the 758-772 nm window (0.1 m⁻² μm⁻¹ sr⁻¹ vs. 0.3 m⁻² μm⁻¹ sr⁻¹ for GOSAT, OCO-2, TropOMI, etc., Fig. 4). Typical SIF values range from 0.0 – 1.8 W m⁻² μm⁻¹ sr⁻¹ (equivalent to a 0-10 gC/m²/day gross CO₂ flux), thus CARBO's enhanced SIF (SIF*) will track variations in SIF (hence GPP) with 5-10% relative precision. This precision is required to investigate the diurnal cycle of fluorescence yield, which links direct to photosynthetic light use efficiency, a key uncertainty in carbon cycle models.

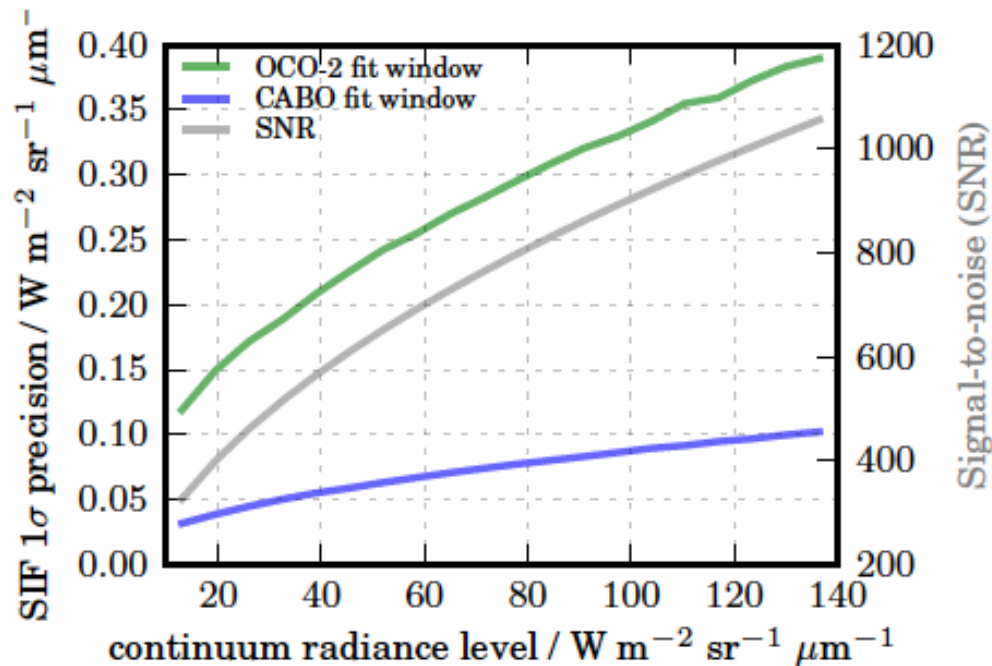


Figure 4. CARBO (blue line) improves SIF detection sensitivity 3-4x compared to OCO-2 (green line) by extending the SIF spectral range to 740 nm. Radiometric simulations indicate that CARBO SIF will achieve better than $0.1 W m^{-2} \mu m^{-1} sr^{-1}$ precision across the expected range of continuum radiance levels.

3. CARBO TECHNOLOGY INNOVATIONS

CARBO advances and matures the key technologies required to create the next generation of space-based greenhouse gas remote sensing instruments. State of the art immersion grating technology lies at the heart of CARBO's innovative spectrometers. Immersion gratings reduce the anamorphic magnification, spherical aberration, and astigmatism that limited the OCO-2 spectrometers. CARBO's immersion grating design yields significantly improved imaging of the FOV on the FPA in both the spectral and spatial dimensions, which in turn enables the use of the entire FPA area even for megapixel (1024x1024 or 1Kx1K) and larger (e.g. 2Kx2K, etc.) FPAs. This translates directly into increased spatial sampling and spectral range with the same spatial- and spectral-resolution as OCO-2 while reducing instrument size and mass. We combine these advantages with state of the art electron beam lithography for exquisite, atomic-level control of the grating groove structure (Fig 5) to reduce stray light below the 10^{-4} level and create polarization insensitive spectrometer response.

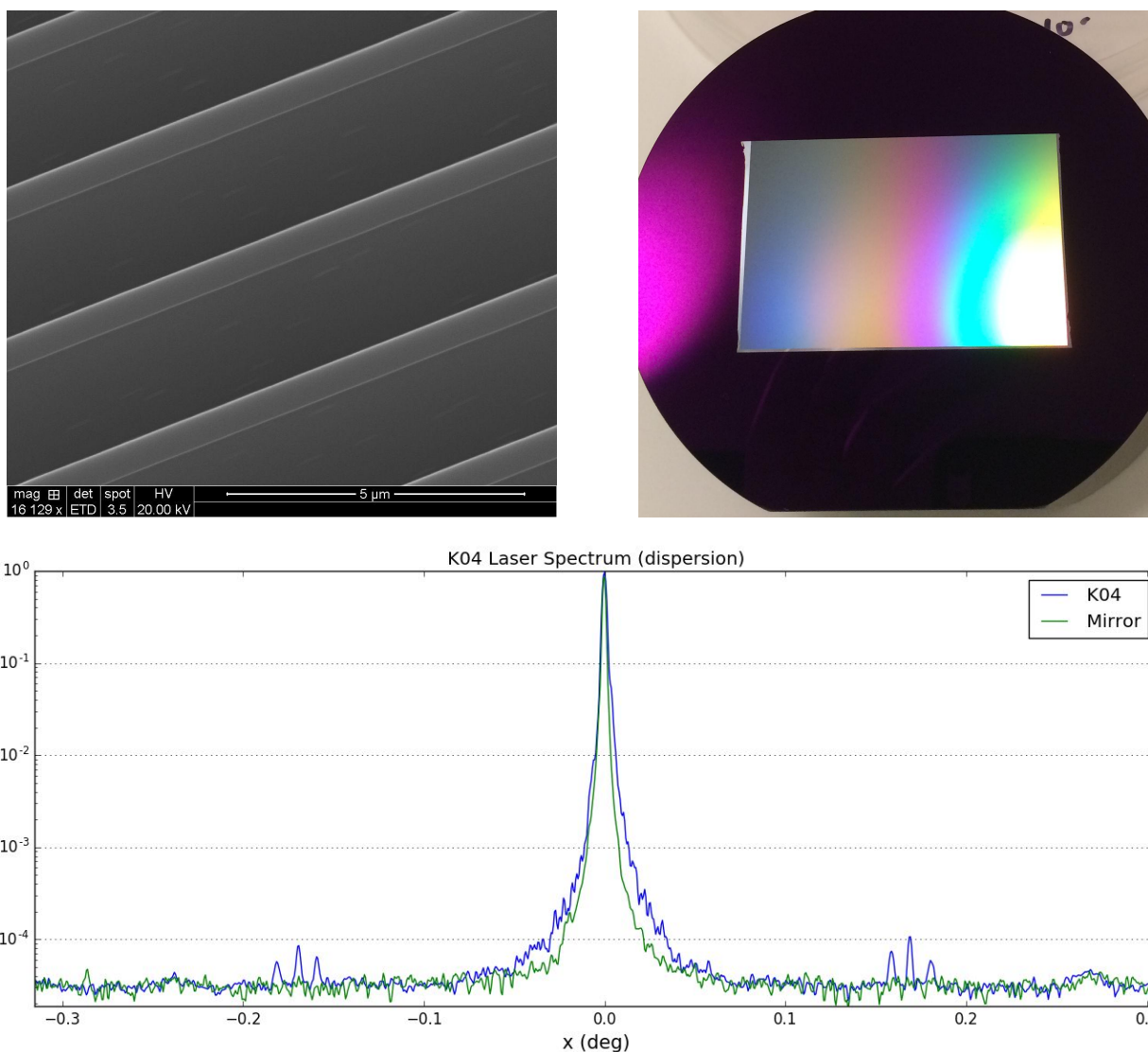


Figure 5. Images of the groove structure, completed prototype grating and stray light characteristics of a Si immersion grating fabricated to CARBO characteristics under the UT/JPL ACT project [34].

CARBO's other major technological innovation is its use of modular channels packaged in structural housings with identical form factors and dedicated telescopes. We required a compact, autonomous, modular architecture to facilitate adaptation to multi-mission needs. CARBO provides scalable system solutions for different measurement and platform requirements. The OCO instrument design - with its monolithic 3-channel housing, common telescope and dichroic beam splitters - made it impossible to increase the number of spectral channels and impractical to simultaneously measure neighboring spectral channels like the $1.65 \mu\text{m}$ CH_4 and $1.61 \mu\text{m}$ CO_2 bands. Our preliminary 4-channel design indicates that the CARBO approach cannot yield the full 30° FOV required for weekly global mapping in each spectral channel. Splitting the target 30° FOV into 15° FOV units for the 2-channel system simplifies the optical design, enables use of reasonably sized immersion gratings ($< 30 \text{ mm}$), improves instrument performance and greatly reduces overall instrument size, weight and cost. A fully functional 4-channel CARBO instrument would fit within the NASA Earth Ventures Instrument (EV-I) cost cap. Specifications of the channels and key requirements are given in **Table 1**.

Table 1. Key CARBO Requirements

CARBO Requirement	Channel 1	Channel 2	Channel 3	Channel 4
Spectral Range (nm)	740 – 772	1598 – 1659	2045 - 2080	2305 - 2350
Measurement Targets	O ₂ ^a , SIF*	CO ₂ , CH ₄	CO ₂	CO, CH ₄ , H ₂ O ^b
SNR @ 5% albedo ^c	> 300	> 350	>150	>100
FWHM (nm)	0.05	0.15	0.10	0.12

^aTarget properties: The O₂ A-band is used for surface pressure, cloud & aerosol properties

^bAlso HDO, H₂¹⁷O and H₂¹⁸O isotopologues as tracers of evapotranspiration and atmospheric mixing

^cStated SNR values are the minimum required for 5% albedo, 60° solar zenith angle observing conditions

Table 2. Key CARBO technology advances, comparison to OCO-2, and descriptions of CARBO scientific and mission benefits relative to current technologies

Technology	...affects...	OCO-2	CARBO	Benefits of CARBO Technology Advances
Wide FOV	Global Coverage	0.15%/day	15%/day	Derivation of regional carbon fluxes on weekly time scales; complete mapping
Immersion Gratings	Grating angles Polarization Sensitivity Instr. Volume	$\alpha \sim 55^\circ$ $\beta \sim 73^\circ$ 100:0 $\sim 0.25 \text{ m}^3$	$\alpha \sim 33^\circ$ $\beta \sim 48^\circ$ 50:50 $\sim 0.11 \text{ m}^3$	Reduction in anamorphic magnification, enhanced throughput No need for active slit alignment, simplified operations and retrieval algorithms Size and cost reduction
4 Spectral Channels	Geophysical Variables	CO ₂ , SIF	CO ₂ , SIF*, CH ₄ , CO	Quantifying the entire carbon budget, disentangling natural and anthropogenic fluxes, source attribution
Channel Modularity	No. Channels, Design flexibility Redesign cost	Partially Modular	Fully Modular	Adding/removing channels without redesign, Redundancy → Risk Reduction (no single point failures), cost reduction on future instrument development

Below we describe CARBO's Immersion Grating and Modular Spectrometer Design technology innovations. Key technological advances plus their scientific and mission-related benefits are listed in **Table 2**.

3.1 CARBO Technology Innovation: Immersion Gratings

CARBO exploits immersion gratings to break the size-resolving power constraints of traditional spectrometer designs [35]. An immersion grating is a diffractive device where the light is incident on the grating from inside a dielectric medium [36]. The reduced wavelength of light in this high-index medium improves performance by increasing the effective phase delay between adjacent grooves by a factor equal to the refractive index. This reduces the required grating size to achieve a desired spectral resolution, and in high index materials like silicon (Si, $n=3.4$), this can result in significantly more compact devices or devices operating at much smaller incidence angles. The UT IGRINS astronomical spectrograph yields diffraction-limited spectra and no measured performance limitations attributable to its

Si immersion grating [37]. CARBO optical designs leverage these properties to achieve >50% reduction in mass and volume compared to OCO-2 while maintaining comparable SNR, spectral- and spatial-resolution and increasing spectral range.

The University of Texas (UT) silicon diffractive optics group produces silicon immersion gratings using microlithographic and chemical etching techniques. Under a recently completed ACT award, the UT/JPL team successfully fabricated prototype silicon immersion gratings with the characteristics appropriate for CARBO channels 2 – 4 (**Fig 5**), significantly reducing CARBO implementation risk [34]. The techniques developed during the ACT task will enable us to fabricate CARBO Si immersion gratings in < 24 months.

Silicon is opaque in the 740–772 nm spectral range and cannot be used for CARBO's Ch. 1. Instead, we will use a glass prism coated with polymer e-beam resist, fabricating grating grooves by grayscale ebeam exposure followed by aqueous-based etching until the desired blaze angle is achieved. This is similar to the processes used by JPL to make the space-qualified gratings for Hyperion (EO-1), CRISM (Mars Reconnaissance Orbiter), ARTEMIS (TacSat-3), and Moon Mineralogy Mapper (Chandrayaan-1). A prototype for the CARBO glass immersion grating (groove period 1.28 μm , blaze angle 39°) was successfully fabricated under a JPL Research & Technology Development task. We verified that it meets the small spectrometer size factor despite its lower index of refraction ($n \approx 1.5$).

3.2 CARBO Technology Innovation: Modular Instrument/Telescope Design

In CARBO's modular architecture each spectral channel is an autonomous unit having its own telescope, optics and detector. The modular concept is achieved by designing all spectral channels to fit in identical housings, which are integrated into an overall instrument assembly. The inclusion of carefully placed fiducials on the individual units will allow mechanical tolerances to ensure the co-alignment requirements are met without the need for extensive and time-consuming alignment procedures at the instrument level. Detailed performance testing can then be done on the individual spectrometers, allowing the use of smaller chambers and simpler optical ground support equipment. This approach maximizes the reuse of alignment fixtures and metrology equipment. A modular concept following this approach could be easily adjusted to varying scientific needs and/or resource constraints without the need to redesign the entire instrument (e.g. descope FOV from 30° to 15° or decreasing the number of spectral channels).

A CARBO design with 15° FOV (bi-weekly global coverage) would weigh <65 kg, <50% of OCO-2 despite a 25-50x swath increase. Conceptual similarities can be observed for instance in the camera design. Two major advantages of CARBO's immersion grating are apparent: 1) the overall spectrometer unit is far smaller despite the larger FOV and 2) the large grating angles in OCO-2 are relaxed in the CARBO design (see **Table 2**), ensuring a more homogeneous optical performance across the entire focal plane array and allowing a polarization insensitive design. These changes increase CARBO throughput, enabling OCO-2 like SNR and eliminate the need for rotating the instrument FOV to align with the principal plane.

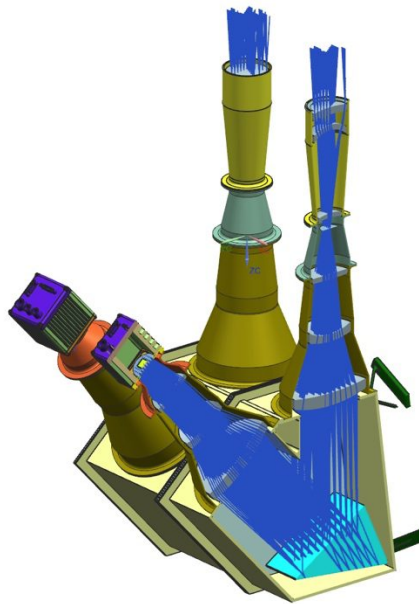


Figure 6. An optomechanical rendering of a 2-channel CARBO spectrometer with a cutaway of one channel to reveal its optical ray trace. Light enters the telescope from the top of the figure, travels through the immersion grating (light blue prism at the base of the spectrometer) and is directed onto the detector (purple cube). All CARBO spectral channels fit within the same modular housing, greatly enhancing the ability to expand or redesign spectrometers for different uses or platforms.

4. COMPARING CARBO TO EXISTING TECHNOLOGY

There is no single current or planned satellite instrument that delivers CARBO's combination of accurate CO₂, CH₄, CO and SIF weekly global mapping at high spatial resolution. The strengths and weaknesses of various approaches are summarized in **Table 3**.

The closest comparison from a technological viewpoint is the TropOMI instrument (LRD late 2016), which will pioneer the immersion grating spectrometer for Earth observations from space [38]. However, TropOMI lacks the critical CO₂ channel, and compared to CARBO its ~7 km x 7km spatial resolution diminishes its sensitivity to point sources by ~12x and decreases its estimated number of cloud free scenes by ~2x [21]. ESA's CarbonSat candidate mission (a traditional grating design) had similar measurement requirements to CARBO, but lacked the CO channel critical for flux attribution, and was considered too much cost risk for EE8 selection. Parametric cost models project CARBO's compact, lightweight design to fall well within the EV-I cost cap, while CARBO's modular nature and use of proven technologies significantly reduces implementation risk. CARBO delivers the essential CH₄ and CO measurements OCO-2 lacks while adding weekly mapping in a more compact, cost-effective package. CARBO nearly matches OCO-2 spectral resolution, spatial resolution, and SNR performance while delivering 3-4x improvement in SIF detection sensitivity. CARBO's polarization insensitive design simplifies operations and enables CARBO to fly on any platform with a dedicated nadir viewing deck.

Table 3. Comparative Technology Assessment of GHG Remote Sensing Satellites

Sensor	CO ₂	CH ₄	CO	SIF	Global Coverage	Fine Spatial Resolution	Weekly Revisit
CARBO	1.5 ppm	7 ppb	5 ppb	<10%	Yes	~2 km	7 days
OCO-2	1.0 ppm	N/A	N/A	30%	~7%	~2 km	16 days
GOSAT	1.5 ppm	30 ppb	N/A	30%	~2%	~10 km	3 days
GHGSat	TBD	TBD	N/A	N/A	TBD	~0.1 km	14 days
TropOMI	N/A	<18 ppb	<10 ppb	30%	Yes	~7 km	7 days
TanSat	1-4 ppm	N/A	N/A	TBC	7% TBC	~10 km	16 days
MERLIN	N/A	10 ppb	N/A	N/A	~1%	50-100 km	16 days
MicroCarb	1.0 ppm	N/A	N/A	TBD	3%	~6 km	16 days
ASCENDS	2.0 ppm	N/A	N/A	N/A	~1%	50-100 km	16 days
CarbonSat	1.2 ppm	7 ppb	N/A	30%	Yes	~2 km	3 days

5. CONCLUSIONS & OUTLOOK

We have presented a preliminary optomechanical design for CARBO, an innovative modular, high-sensitivity remote sensing instrument designed to deliver weekly global maps of CO₂, CH₄, CO and SIF from low Earth orbit. CARBO fills a critical gap in the Earth Science satellite program [39-43] and advances key technologies – immersion gratings and a modular design – to enable high-performance, cost-effective solutions for a carbon-climate observing system. Additionally, its compact, low-mass design opens up options for deployment on platforms ranging from smallsats to the International Space Station. Work continues to develop ground-based and airborne versions of CARBO to fully demonstrate these technologies and validate measurements from the current generation of greenhouse gas satellite sensors.

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